2016 KIVA-hpFE Development: A Robust and Accurate Engine Modeling Software

David Carrington
Los Alamos National Laboratory

June 7, 2017

11:00 a.m.

This presentation does not contain any proprietary, confidential, or otherwise restricted information
LA-UR-17-23370

Project ID # ACS014

Overview

Timeline

- 10/01/09
- 9/31/18
- 85% complete (the last 10% in CFD development takes the most effort)

Barriers

- Minimization of time and labor to develop engine technology
  - User friendly (industry friendly) software, robust, accurate, more predictive, & quick meshing
- Improve understanding of the fundamentals of fuel injection, fuel-air mixing, thermodynamic combustion losses, and in-cylinder combustion/ emission formation processes over a range of combustion temperature for regimes of interest by adequate capability to accurately simulate these processes
- Engine efficiency improvement and engine-out emissions reduction

Budget

- Total project funding to date:
  - 4500K
  - 500K in FY 17
  - subContractor (Universities)~15%

Partners

- Dr. Jiajia Waters, LANL
- Brad Phillipbar, LANL GRA
- University of New Mexico- Dr. Juan Heinrich
- Oakland University - Dr. Peng Zhao
- John Deere – Dr. Haiwen Ge
- Reactive-Design/ANSYS – ChemKin-Pro
- Program Development Company - GridPro Inc.

FY 10 thru FY 16 KIVA-Development

- **Everything we are doing in R&D is to develop methods and a code for:**
  - **Robust, Accurate and Efficient Algorithms in a Parallel (MPI) Modular Object-Oriented code for Industry and Researchers to meet:**
    - **Relevant** to accurately predicting engine processes. To enable better understanding of: fuel injection, fuel-air mixing, thermodynamic combustion losses, and in-cylinder combustion/ emission formation processes. Ranges of physics regimes spanned with adequate capability for accurately simulating these processes.
      - **More accurate modeling requires new algorithms and their correct implementation.**
        - Developing more robust and accurate algorithms with appropriate/better submodeling
          - Relevant to understand better combustion processes in internal engines
        - Providing a better mainstay tool
          - Relevant to improving engine efficiencies and
          - Relevant to help in reducing undesirable combustion products.
        - Newer and mathematically rigorous algorithms will allow KIVA to meet the future and current needs for combustion modeling and engine design.
  - **Easier and quicker grid generation**
    - **Relevant to minimizing time and labor for development of engine technology**
      - CAD to CFD via GridPro or Cubit Grid Generation Software
      - KIVA-4 and KIVA-3v engine grid generation with GridPro
      - Easy CAD to CFD using GridPro or Cubit grid generator - *hp*-FEM CFD solver with overset actuated parts and new local ALE in CFD, removes problems with gridding around valves and stems.

Objective

2017 DOE
Merit Review

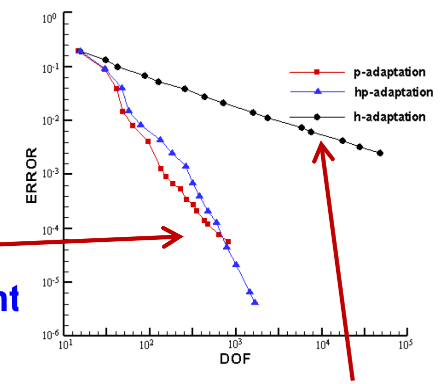
More Predictive Turbulent Reactive Flow Modeling in Engines

(most of the following attributes are those heralded by industry as necessities)

RED highlight subjects are discussed here-in

1) **Great dynamic LES, well suited for engine flows**
2) **Computational speed with MPI** for parallel processing
   a) 300x speed-up and is Super-linear
   b) *Minimal communication* for faster parallel processing
   c) Exascale possibilities because most operations are local to elements
   d) GPU friendly CFD
3) ***Predictive spray modeling***
4) ***Robust moving immersed parts*** *2nd order accurate Local ALE*
5) ***Fast grid generation*** **- CAD to CFD** grid in nearly a single step
6) ***Great reactive chemistry of ChemKin-Pro (so far)***
7) ***Accurate Spray modeling – spatially convergent,***
8) *Higher order accurate* - *hp*-adaptive FEM – exponentially grid convergent
9) **3rd order accurate advection**, very important for species and heat transfer
10) Surfaces are represented exactly
11) ***Evolving solution error drives grid***
12) **Eulerian Solve throughout**
13) **Good RANS *k-ϖ* turbulence modeling**
14) ***Conjugate Heat Transfer (CHT)***
15) **Plasma Spark Model applied at the element node**
16) **A software for industry via commercialization and collaboration**

hp-adaptive **FEM**
– exponential grid convergent



Error as function(*grid size*)
Typical CFD method

Milestones for FY16 (& thru March 2017)

04/16 – Parallel Moving Parts complete with compressible flow KIVA-hpFE

06/16 – Implicit Parallel solution speed-up test case of flow over a cylinder

07/16 – DISI Engine grid created for use KIVA-4 finite volume method

08/16 – *hp*-adaptive system working in updated compressible flow algorithm

09/16 – KIVA-3V and KIVA-4 format support in GridPro

11/16 – *GridPro* to KIVA-hpFE file converter routines constructed for KIVA-hpFE

12/16 – *ChemKin-Pro* linking subroutines and entire model compiled and linked

01/17 – Vertical valve engine test grid constructed with GridPro using overset parts

02/17 – Low Mach algorithm adjustment concepts for intake stroke

02/17 – Low Mach compressible flow LES test flow over a cylinder are high Re

03/17 – Predictive spray break-up – VOF for incompressible liquids combined with compressible gas

04/17 – Parallelizing *hp*-adaptive system (ongoing) for effective 3-D simulations

03/12 to 02/17 –
Presentations at SAE, AEC, ASME, ICHT, IHTC
Papers to ASME, ICHT, IHTC, NHT, and CTS

Approach to achieve Objectives

- **Design** and **Invent new modeling, methods** and software
  - The **new Design** is change of discretization to FEM method
  - The FEM allows for many improvements:
    - Invent the FEM PCS projection method
    - Develop the *hp*-adaptive system
    - Invent the local-ALE method more moving bodies
    - Develop new Dynamic LES,
    - Invent Method for fast parallel solution on today's & future platforms.
    - Develop Volume of Fluid for Predictive Spray Injection Primary Break-up
    - Implement high-fidelity chemistry packages (ChemKin-Pro to date)

– *Design, Invent, Develop, Implement, Validate, Verify…*

Build the models and code so that it meets all the objectives

- Build the model in new Fortran, objective, clean, easy to maintain and add submodels
- Careful Verification and Validation on pertinent problems

Technical Accomplishments - overall

New Methods and Models for more Predictive Modeling

***FEM* Flow modeling**

- ***Implicit Solution Algorithm and linear equation solvers fully implemented***
- ***KIVA-FEM is faster and more accurate than FVM KIVA-4***
- ***Predictive Spray modeling, Volume of Fluids (VOF) for primary break-up***
- **Dynamic LES** capable of transitioning from laminar to fully turbulent flow
- ***Chemistry and Fuels incorporated (ChemKin-Pro added)***
- *More Accurate droplet transport modeling*
- *Eulerian solution frame*
- *Spark Plasma Kernel Approximation, engineering model based on ODE solves*
- *Conjugate Heat Transfer method being developed (maybe too with Boundary Element coupling)*

hp-adaptive FEM

- **Higher order accurate** - 2^{nd} and higher, minimum **3^{rd} order accuracy advection terms**
- *Evolving solution error drives grid*
  - Resolution and higher-order approximation
- ***hp*-adaptive FEM – exponentially grid convergent**

Local ALE in FEM

- ***Quick, accurate, robust moving parts (Mesh can never tangle)***
  - ***Robust and 2^{nd} order accurate Local ALE for moving parts!***
- ***Overset parts for must faster grid generation*** - CAD to CFD grid in nearly a single step

Grid Generation

- *Faster grid generation with GridPro and Cubit (for all KIVA codes)*

Parallel Solution

- **Minimal communication for faster processing – Super linear speed-up**
- ***Efficient MPI and OpenMP processing on moderate computer platforms.***

RED highlight subjects are discussed here-in

And a great many more win-win & win-win-win improvements

Technical Accomplishments in 2016 (thru March 2017)

KIVA-hpFE for *achieving robust, efficient, & accurate Engine Modeling*

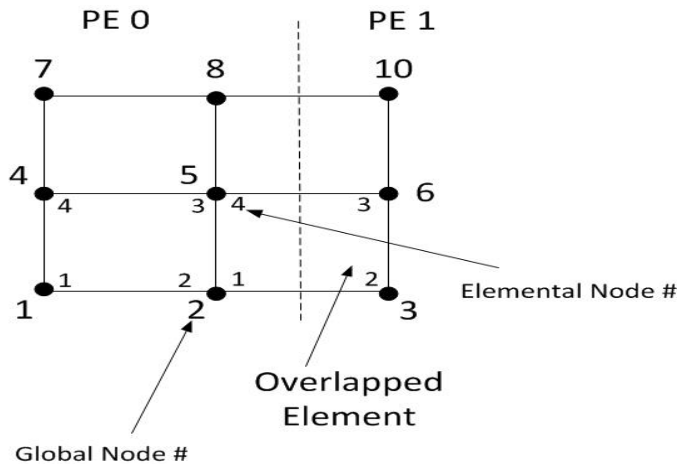
- ***Implicit Solution***
  - **Larger time step size – up to 1000x larger than explicit method and is faster than explicit**
  - **Implicit Viscosity & diffusion, explicit advection (for 300x overall speed-up)**
- ***Dynamic LES turbulence modeling***
  - ***LANL's LES has the following attributes (must haves for accurate engine modeling)***
    - ***Spans laminar to fully turbulent flows***
    - ***Wall bounded flows without need for wall-law functions***
- ***Parallel Solution***
  - ***Efficient MPI processing for moderate to LANL type computer platforms.***
    - **By design - Minimal communication for faster processing – 300x speed-up & Super-linear!**
    - ***Much faster vs. previous Finite Volume KIVA codes – our FEM is faster than our FVM***
- ***hp-adaptive FEM exponentially convergent > p > 2***
  - ***Revamping the hp-adaptive system for memory efficiency***
  - ***Parallelizing the adaptive algorithms***
- ***Spray modeling enhancement with VOF system***
  - ***Predictive Spray modeling, true multi-phase flow modeling***
- ***Reactive Chemistry***
  - ***ChemKin-Pro interface system constructed, compiled and linked***
- ***Local-ALE in FEM methods***
  - ***never been done before - the most difficult invention but,***
    - ***2nd order spatial accuracy***
    - ***Allows for fast grid generation, takes only 1% of solver time to move parts***

Dynamic LES for wall-bounded and transitional flow

- **LANL's KIVA-hpFE LES**
  - Laminar to turbulent, method handles transitional flow
    - **Required for engines, not always turbulent, and is certainly wall-bounded flow**
  - Self-damping at wall, no law-of-the-wall (required for accurate modeling)
- **Dynamic LES**
  - Backscatter (upscaling of small eddy energy to larger scales)
  - Results on coarse grids similar to k-ϖ RANS
  - Validated with experimental data on pertinent problems
  - The DSGS model calculates the model coefficient from the energy of the smallest resolved scale
  - Governing Navier-Stokes and transport equations become filtered equations

Parallel Solution of the Implicit Diffusion/Viscous Predictor-Corrector Scheme

- Two sets of decomposition: one for the elements and one for the nodes
  - Read an element and processor file (par-metis to decompose the mesh)
  - Use the element and processor file to generate a node and processor file.
- The integration over an **overlapped element** requires gathering values whenever a node value is off processor.



Non-overlapped grid portion and an overlapping element portion of the domain

Implicit Viscous solver for Projection FEM

- Implicit viscous terms -- alterations to the Velocity Predictor
- Developed by solving U* implicit viscous terms with explicit advection
- Then extract Δ U* from U*
- Requires greater linear solver resources but is only CFL # limited
  - More work but dt (time step) increase by 10x – hence 300x serial explicit

Governing equations for Implicit Viscous Predictor Corrector Scheme (IVPCS)

$$\rho^n u_i^* - \Delta t * \left(\frac{\partial t_{ij}^*}{\partial x_j} - \frac{\partial \tau_{ij}^*}{\partial x_j} \right) = \rho^n u_i^n - \Delta t * \frac{\partial \left(\rho^n u_i^n u_j^n \right)}{\partial x_j}$$

where $t_{ij}^* = \mu \left(\frac{\partial u_i^*}{\partial x_j} + \frac{\partial u_j^*}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial u_k^*}{\partial x_k} \delta_{ij}$ $\quad \tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\mu_{sgs} \left(\tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right)$

and $S_{ij}^* = \frac{1}{2} \left(\frac{\partial u_i^*}{\partial x_j} + \frac{\partial u_j^*}{\partial x_i} \right)$

$\left\{ U_i^* \right\}$ is an intermediate prediction of velocity u

where $\left\{ \Delta U_i^* \right\} = \left\{ U_i^* \right\} - \left\{ U_i^n \right\}$

Conservative IVPCS solver for all flows

- Solve pressure in usual manner
- Specific internal energy is solved again in implicit form

$$E^{n+1} - \Delta t \times \frac{\partial}{\partial x_i}\left(\frac{\kappa}{C_v}\frac{\partial E^{n+1}}{\partial x_i}\right) - \Delta t \times \frac{\partial}{\partial x_i}\left(\frac{C_p \mu_{sgs}}{\Pr_{sgs} C_v}\frac{\partial E^{n+1}}{\partial x_i}\right) =$$
$$E^n - \Delta t \times \frac{\partial}{\partial x_i}\left(E^n u_i^{n+1} + P^{n+1} u_i^{n+1}\right) + \Delta t \times \frac{\partial}{\partial x_i}\left(t_{ij}^{n+1} + \tau_{ij}^{n+1}\right)$$

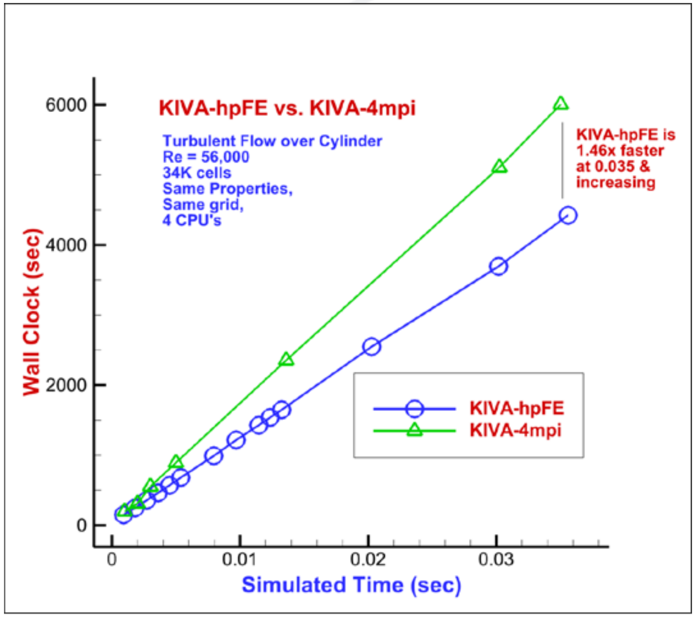
Here $E^{n+1} = \rho^n e^{n+1}$ and e^{n+1} is the internal energy

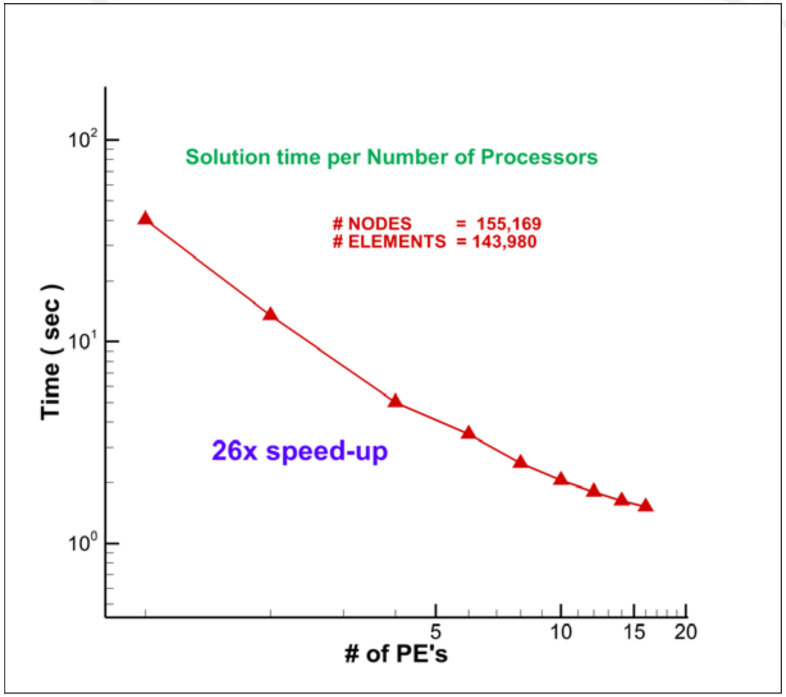
Temperature $T^{n+1} = \dfrac{e^{n+1}}{C_v}$

Species transport equations

$$\rho^n \Upsilon_j^{n+1} - \Delta t \times \frac{\partial}{\partial x_i}\rho^n\left[\left(D_{j,N} + \frac{\mu_{sgs}}{Sc_t}\right)\frac{\partial \Upsilon_j^{n+1}}{\partial x_i}\right] = \rho^n \Upsilon_j^n - \Delta t \times \frac{\partial}{\partial x_i}\left(\rho^n u_i^{n+1} \Upsilon_j^n\right)$$

Comparison of KIVA-4mpi to KIVA-hpFE
Parallel implicit solver systems





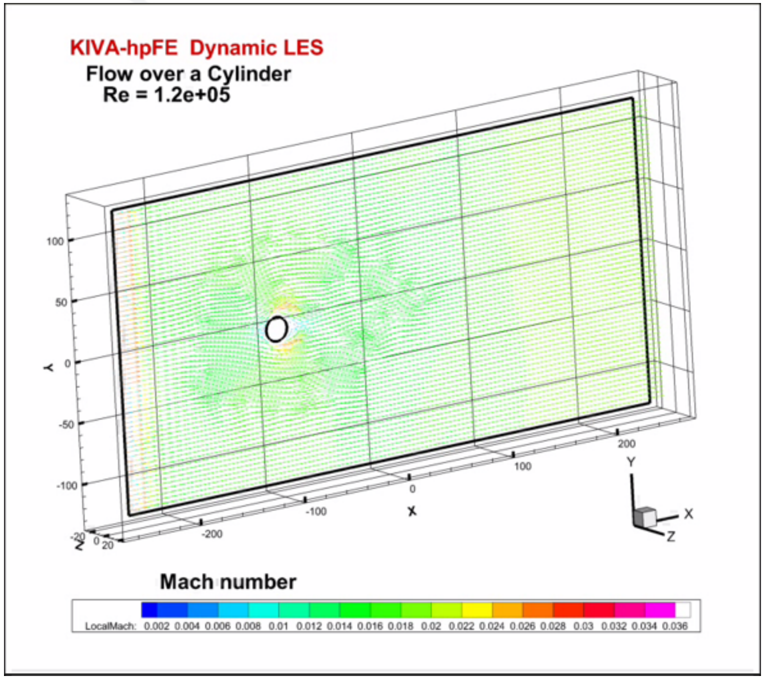
- KIVA-hpFE FEM vs. KIVA-4mpi
  - FEM versus Finite Volume (FVM)
  - Same computer, #CPU's, grid & properties
  - FEM KIVA is faster with continuously ever increasing advantage over FVM method KIVA4! **First for FEM > FVM**
- **FEM is more accurate on same # cells**

- The parallel speed-up is super-linear!

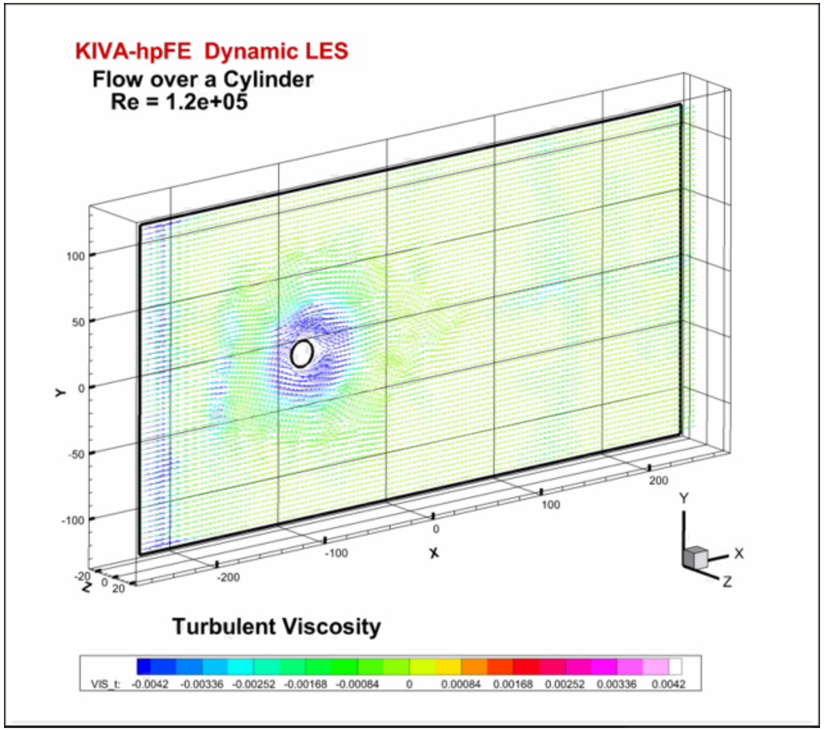
Implicit LES - 3D Flow over a cylinder

- 300x speed-up over FEM serial version
- 10x faster than explicit MPI FEM
- Must faster than KIVA-4 parallel
- More Accurate than KIVA-4 with fewer cells
- 8 CPU's 14K nodes/CPU -> 112K nodes
- 9 m/s inlet velocity, compressible flow

Local Mach #



Turbulent viscosity



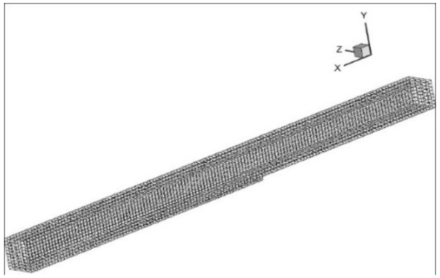
Low Mach Flow

Compares very favorably to experimental data

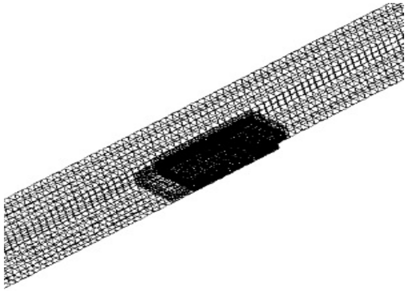
3-D Flow over a Backward-Facing Step using Parallel h-adaptive FEM with LES

- Compressible flow solver having Re ~ 26.5K
- Step height ratio to inlet = 1:8
- Zero gradient at outflow boundary, no-slip boundary conditions on the walls except for the Z direction which receives a periodic boundary condition to remove the 3D effects from the side walls.
- The initial mesh starts having 6955 nodes and 4976 elements
- After adapting twice the final grid is 19248 nodes and 16596 elements.

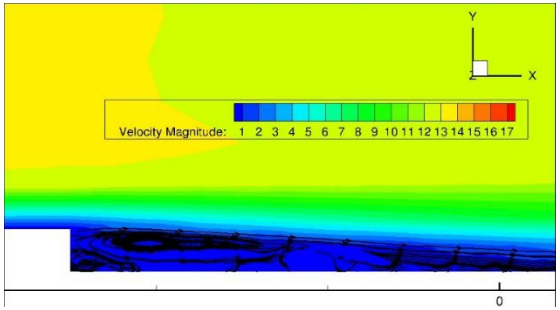
Study problem to help Converge, Inc. understand problems in Convergent



Initial mesh



Final mesh

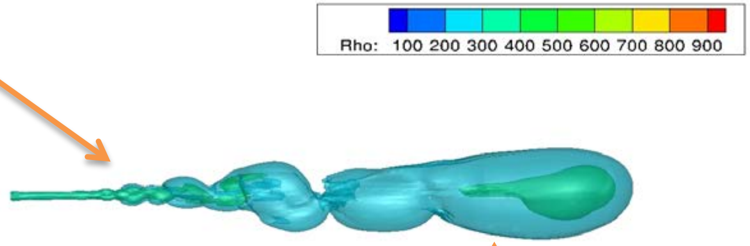


Velocity behind step

UNCLASSIFIED

Injection / Spray Modeling
Volume of Fluids Method

- Spray Modeling - Predictive Liquid Jet Break-up into Droplets
  - Methods being developed
    - Primary break-up
      - Volume of Fluids (VOF) for interface tracking of liquid jet core & ligaments
      - Combined with h-adaptive system to improve resolution minimize computational cost
      - Interface break-up via complete stress modeling,
        - liquid core transforming to ligaments



    - Lagrangian Particle Transport
      - Hand-off primary break-up, small ligaments to Droplet Transport (low density envelope)
        - Ligaments are small enough for atomization modeling to be effective
    - Tabularized size distribution to feed Engineering KH-RT model
        - For Engineering coarse grain simulations

VOF System with LES

VOF: f is the Volume of Fluids(VOF)

$$\frac{\partial f}{\partial t} + U \cdot \nabla f = 0$$

Integrate f on each element to get the elemental value for f:

$$fE = \frac{\int_e f\, dV}{V_e}$$

Momentum: Fractional Split method

If *f=1*, run incompressible equation.

$$\frac{\rho^n u_i^* - \rho^n u_i^n}{\Delta t} = -\rho^n U \cdot \nabla u_i + \left(\mu + \mu_{sgs}\right)\frac{\partial^2 u_i}{\partial^2 x_j} + \delta\kappa n \delta_\Gamma$$

If *f≠1*, run compressible equation.

$$\frac{\rho^n u_i^* - \rho^n u_i^n}{\Delta t} = -\rho^n U \cdot \nabla u_i + \frac{\partial t_{ij}}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \delta\kappa n \delta_\Gamma$$

where u_i^* is the intermediate velocity, δ_Γ is a Dirac Delta function on the interface.

VOF System Surface Tension

Surface tension: (FEM)

Multiplying by a test function v

$$\int_{\Gamma} \sigma \kappa \hat{n} \delta_{\Gamma} \cdot v$$

where κ in surface curvature, σ is surface tension,

when the interface is smooth enough:

$\nabla f = n\delta_{\Gamma}$ by setting $\delta_{\Gamma} = |\nabla f|$ and $n = \frac{\nabla f}{|\nabla f|}$

this is valid in the volume domain:

$$\int_{\Gamma} \delta \kappa n \delta_{\Gamma} \cdot v = \int_{\Omega} \delta \kappa \nabla f \cdot v$$

- When f is discontinuous, special care has to be taken to get ∇f
- Due to FEM, f is continuous for each element. Easy to calculate ∇f
- No need to track the interface because of ∇f

VOF System Pressure Solve

Pressure solve:

$$\frac{1}{c^2}\Delta P - \Delta t^2\theta_1\theta_2\frac{\partial^2\Delta P}{\partial^2 x_i} = \Delta t^2\theta_1\frac{\partial^2 P^n}{\partial^2 x_i} - \Delta t(\theta_1\frac{\partial\Delta u^*}{\partial x_i} + \frac{\partial\rho^n u_i^n}{\partial x_i})$$

compressible flow: sound speed $c = \sqrt{\gamma RT}$

incompressible flow: we use artificial compressibility

match the time step in incompressible with compressible

$$c = \beta = \max(\varepsilon, u_{conv}, u_{diff})$$

Pressure not continuous,

solve $\frac{\int_{cv} p\,dv}{V}$ to get pressure for the control volume for $0 \le f < 1$

Gas density: If $0 \le f < 1$, $\rho_{gas} = \frac{P}{RT}$

VOF System Energy and Species with LES

Energy: $f > 0$, solve incompressible equations for internal energy E:

$$\rho_{liquid}\frac{\partial E}{\partial t} = -\rho_{liquid}C_{p,liquid}U \cdot \nabla T + \frac{\partial}{\partial x_i}\left(\kappa_{liquid} + \frac{C_{p,liquid}\mu_{sgs}}{Prt_{sgs}}\right)\frac{\partial T}{\partial x_i}$$

$f = 0$, solve compressible equations for internal energy:

$$\rho_{gas}\frac{\partial E}{\partial t} = -\rho_{gas}U \cdot \nabla E - P\nabla \cdot U + \frac{\partial}{\partial x_i}\left(\kappa_{gas} + \frac{C_{p,gas}\mu_{sgs}}{Prt_{sgs}}\right)\frac{\partial T}{\partial x_i} + \frac{\partial}{\partial x_i}(t_{ij} + \tau_{ij})u_j$$

Species: solve only on gas species, mass fraction : $\Upsilon_j = \frac{\rho_j}{\rho_{gas}}$. Liquid density is tracked according to VOF. When $f \neq 1$

$$\rho_{gas}\frac{\partial \Upsilon_j}{\partial t} = -\rho_{gas}U \cdot \nabla \Upsilon_j + \frac{\partial}{\partial x_i}\rho_{gas}(D + \frac{\mu_{sgs}}{Sct})\frac{\partial \Upsilon_j}{\partial x_i}$$

Use γ_i aggregate the gas properties e.g. $C_{p,gas}$, $C_{v,gas}$, κ_{gas} and μ_{gas}

Aggregate the properties by VOF (in momentum only):

$$\mu = f \times \mu_{liquid} + (1-f) \times \mu_{gas} \qquad \rho = f \times \rho_{liquid} + (1-f) \times \rho_{gas}$$

Surface tension test – a validation exercise

3D drop in static equilibrium:

The exact jump in pressure: $\Delta P_{exact} = \sigma \kappa$ and $\kappa_{exact} = 2/R$ in 3D

Domain is a cube having side lengths of 8 units. Grid is $40 \times 40 \times 40$

The drop is at the center with radius R=2. Surface tension $\sigma = 73$

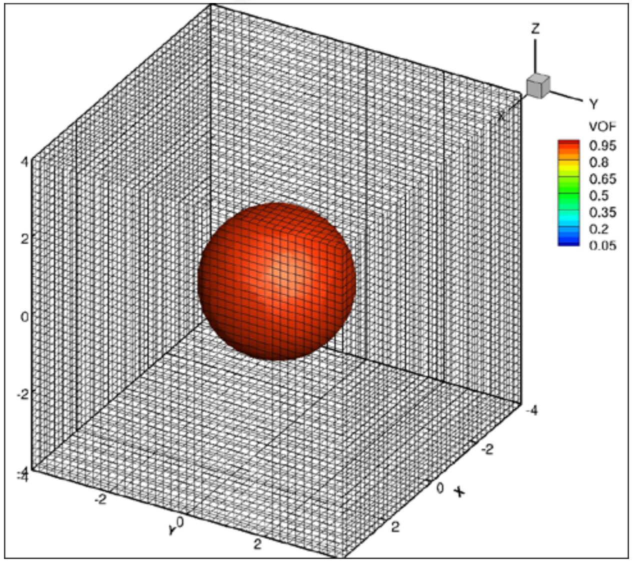
Density inside the drop ρ_2 , background ρ_1 density ranges from 1 to 0

Exact curvature	After one time step		Steady state	
ρ_1 / ρ_2	$\lvert U \rvert_{\max}$	$E(\Delta P_{\max})$	$\lvert U \rvert_{\max}$	$E(\Delta P_{\max})$
10^3	4.6273×10^{-4}	6.2×10^{-2}	1.2386×10^{-3}	2.1918×10^{-4}
10^5	5.3053×10^{-2}	4.72×10^{-2}	1.2178×10^{-1}	3.411×10^{-4}

$$E(\Delta P_{\max}) = \frac{\lvert \Delta P_{\max} - \Delta P_{exact} \rvert}{\Delta P_{exact}}$$

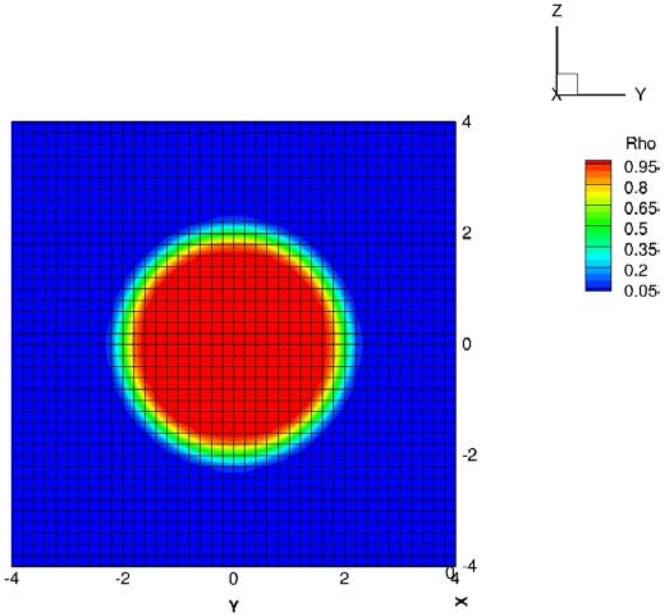
Surface tension test

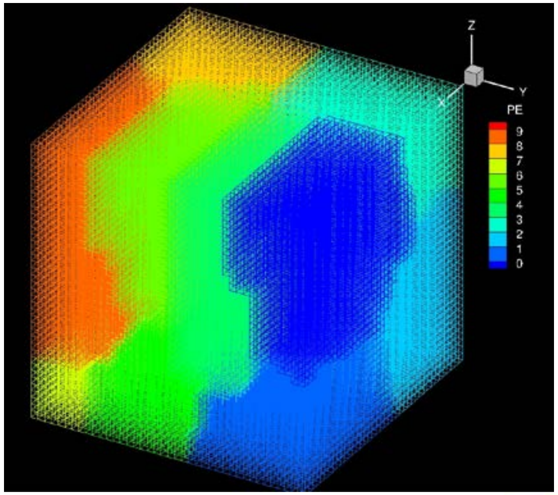
3D static drop:



Static drop in the center (shown as VOF)

2D slice static drop (shown as density)

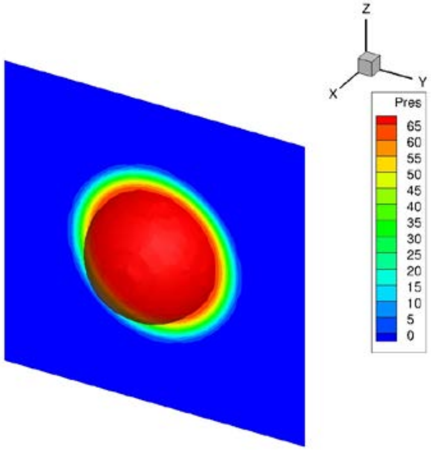




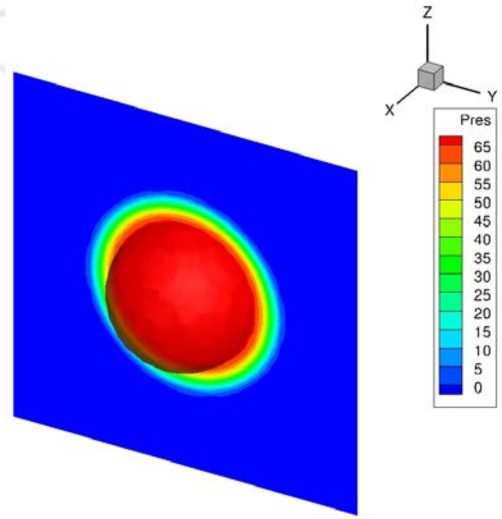
Mesh distributed to 10 CPUs

$40 \times 40 \times 40$

Surface tension test

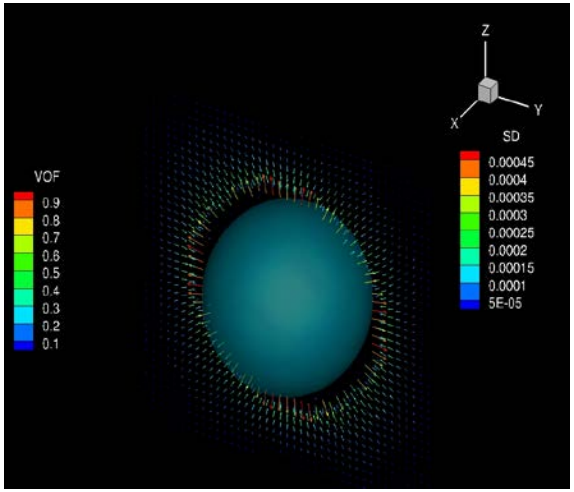


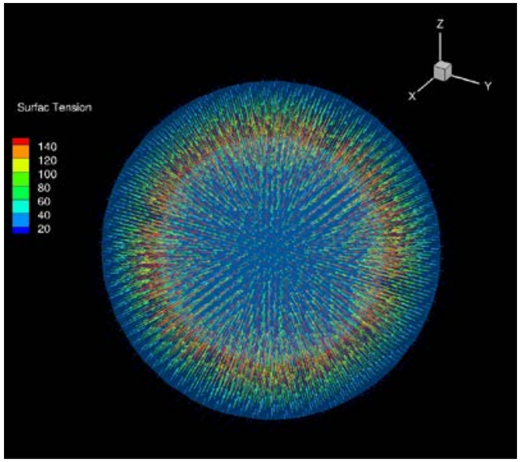
Exact curvature



Pressure for density ratio 10^3 Pressure for density ratio 10^5

Speed and surface tension for density ratio 10^3





Primary break up modeling

Test case material properties*

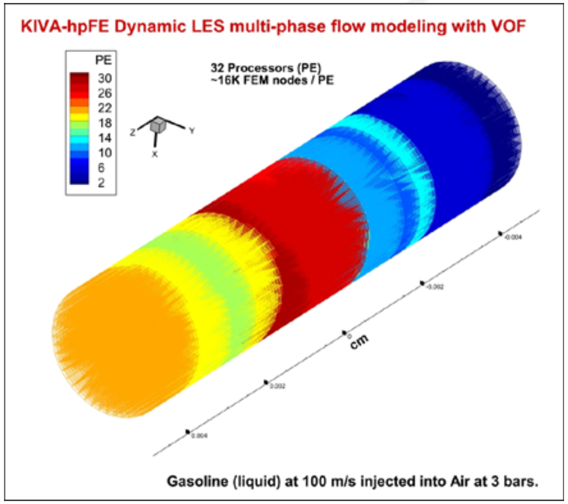
Nozzle diameter D (mm)	Ambient Pressure P (Mpa)	Gas Density kg/m^3	Liquid density kg/m^3	Liquid viscosity (Pa s)	Gas Viscosity (Pa s)	Surface tension Coefficient (N/m)
0.1	3	37.25	931.32	2870e-6	18.465e-6	30.0e-3

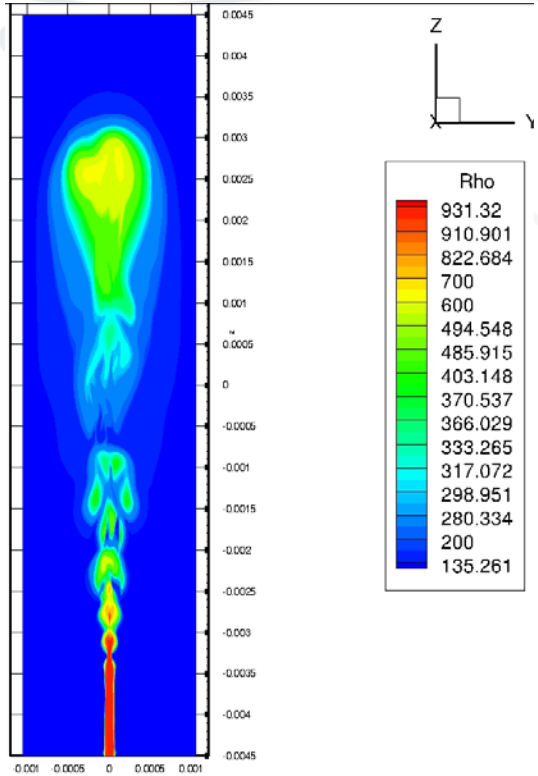
Liquid velocity: 100m/s
Gas velocity: 0m/s
Domain is cylinder with a diameter of 2.31mm and a height of 9.9mm.
93,931 nodes and 90240 elements on to 10 processors

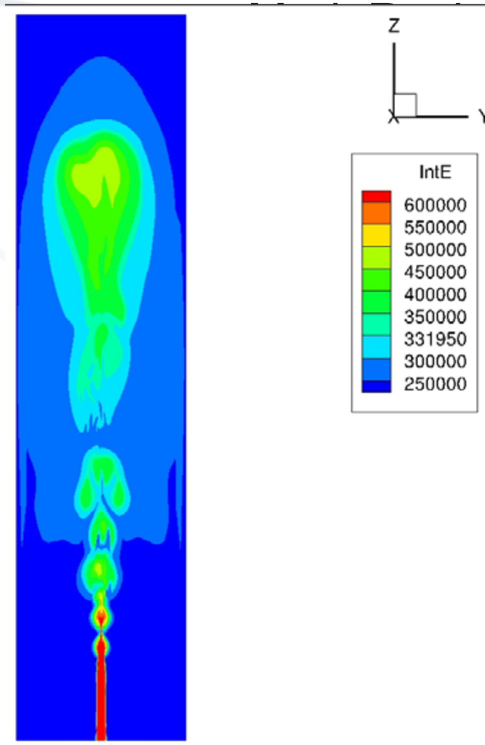
***Shinjo, J., Umemura, A., 2010, Simulation of liquid jet primary breakup: Dynamics of ligament and droplet formation, International Journal of Multiphase Flow, Vol 36, no 7, pp. 513-598, Elsevier**

Predictive Spray Modeling

Primary break-up



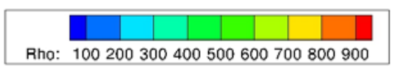


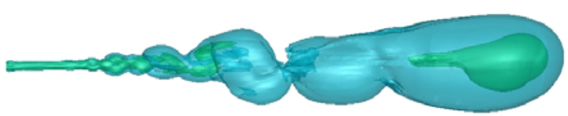


Domain decomposition
32 processors, ~16K nodes per

Density at meridional plane

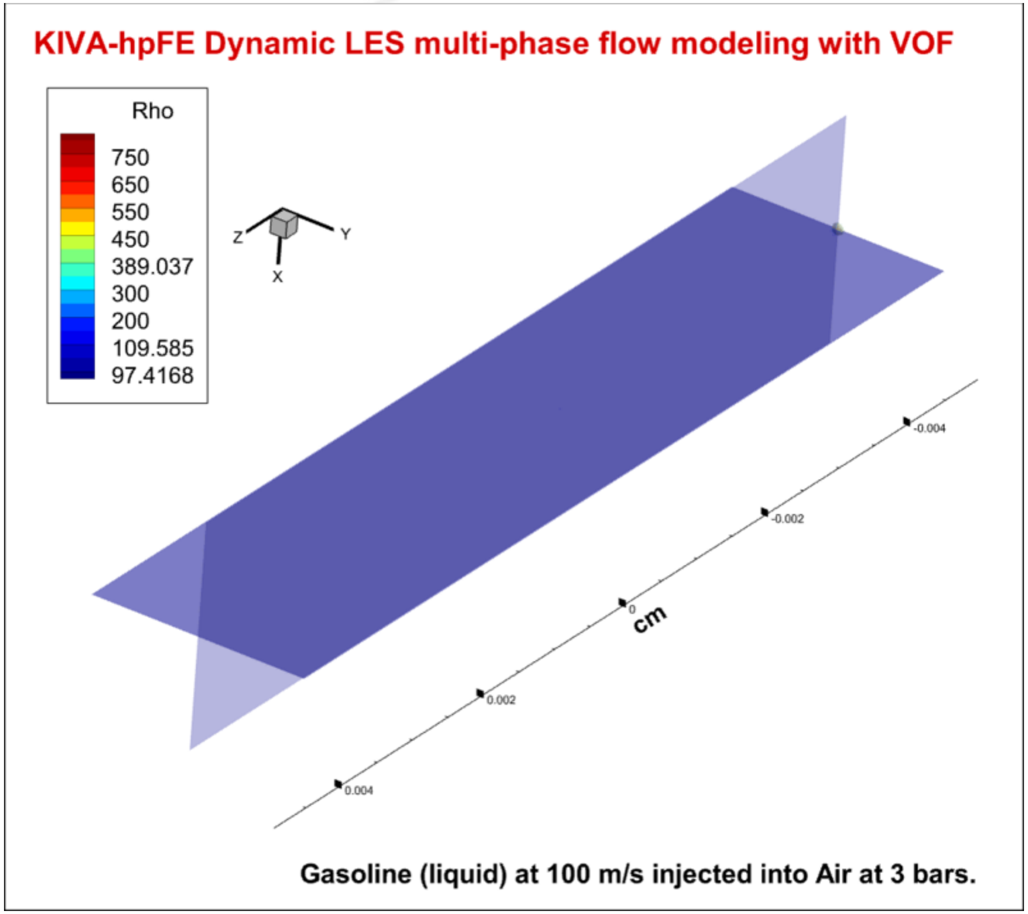
Internal energy at meridional plane

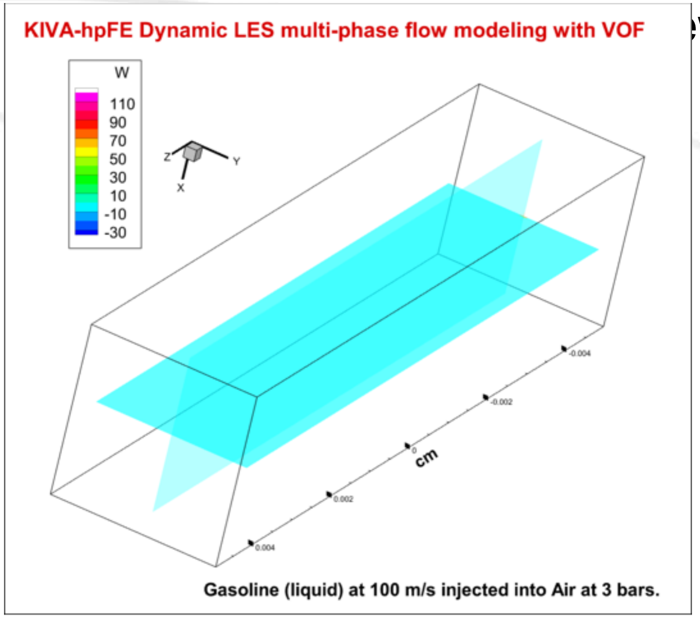




Density of liquid and liquid air mixture

Predictive Primary Spray break-up

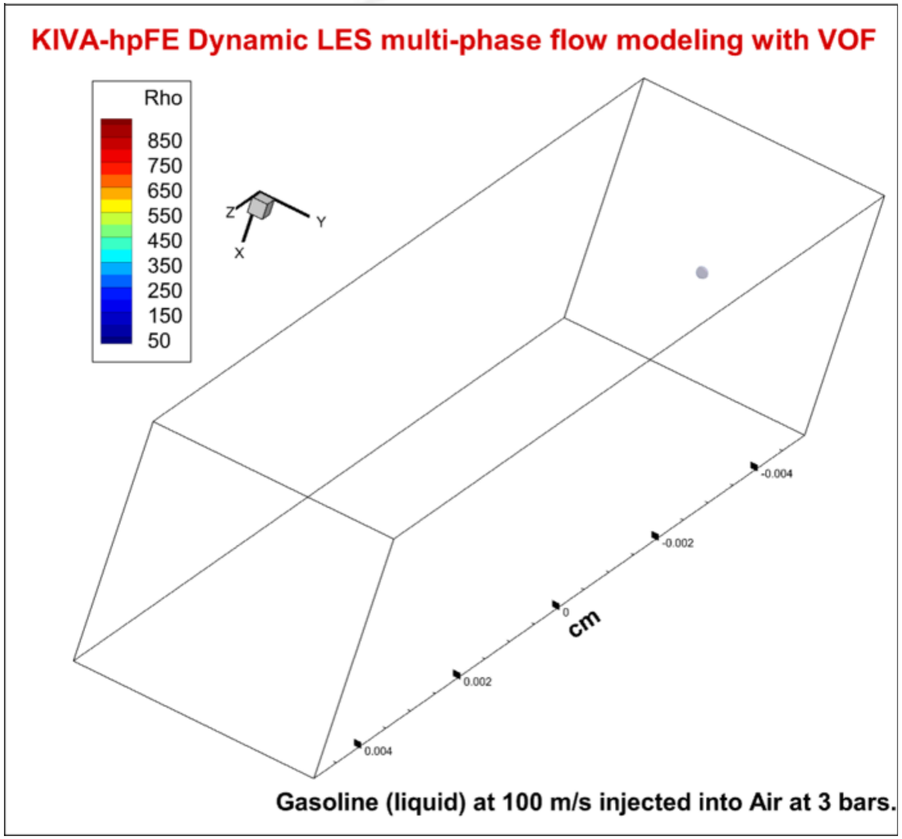




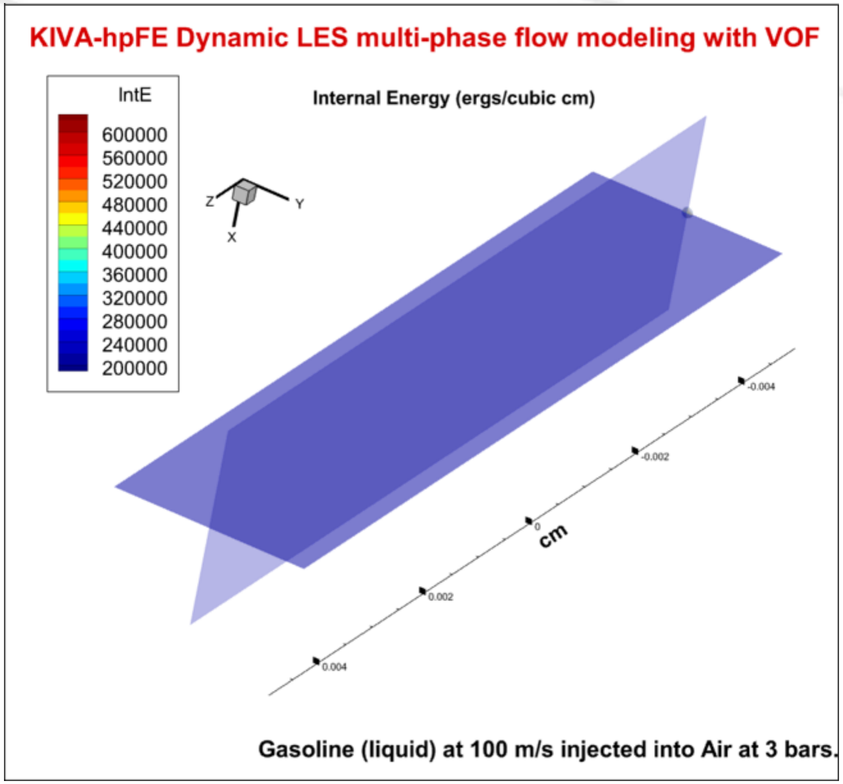
W component of velocity

Density of liquid and mixture during break-up

Predictive Primary Spray break-up



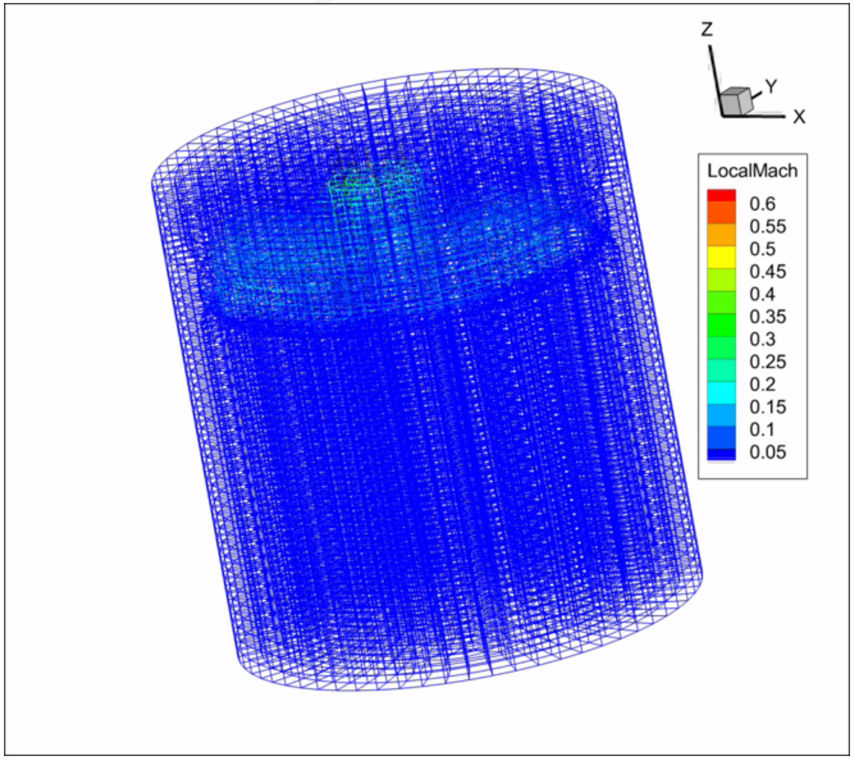
Density of liquid and mixture during break-up



Internal Energy during break-up

KIVA-hpFE Parallel Implicit LES solve

Local 3-D ALE for moving parts on unstructured grids



Local Mach

Curve or Scalloped Bowl Test

- Compressible Flow
- Low Mach to Subsonic
- Unsteady Turbulent Flow

Scalloped Piston Engine Geometry at 1000 rpm

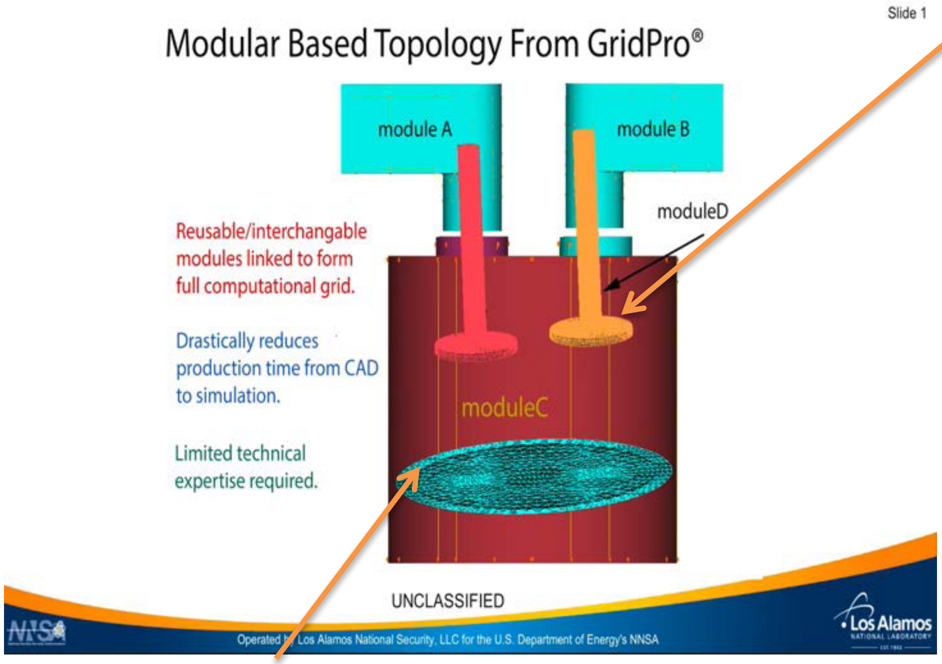
- Dynamic LES is implemented
- **Only 1% of CPU time for grid movement**

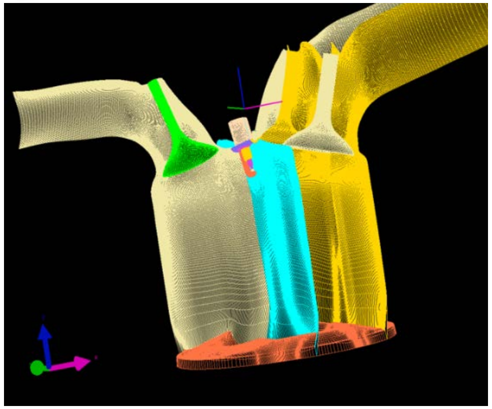
Grid Generation

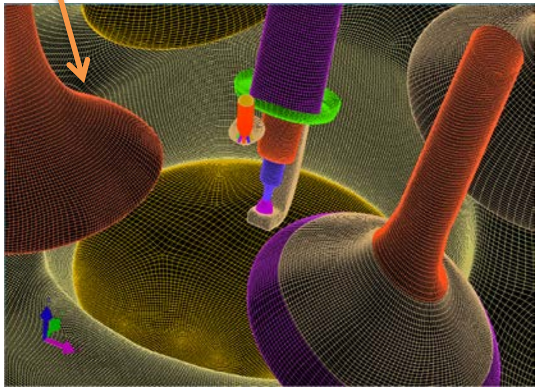
- Overlaying parts for easy/automatic grid generation.

  New Local ALE method allows for Overset grid generation – fast CAD to CFD grid
  - Labor not nearly as significant as traditionally done
  - Robust and Accurate moving parts representation
  - Collaborating with Peter Eiseman at GridPro Inc. KIVA versions now supported

Overlaid valves







Overlaid piston

Sandia DISI engine
From stl surface
by X-ray - Magnus Sjoberg’s engine

Challenges and Barriers

- Challenges include:
  - Turbulence modeling
    - HPC with LES and combustion/spray modeling
    - LES with combustion modeling
  - Better spray modeling, primary break-up and interface capture
    - Two-phase turbulent flow for wall film and primary break-up
      - VOF Interface tracking with solution of interface stress
    - Better Dispersed Spray modeling
  - Full-up engine modeling with KIVA-hpFE
  - Conjugate Heat Transfer seamlessly with parts and engine block
    - Meshless Method Condition model combined with FEM CFD
- Barriers include:
  - Proper sub-modeling of the primary break-up and turbulence along with interface tracking system for two-phase flow.
  - Combustion modeling with LES – interface tracking
  - Heat Transfer to the engine block and parts
    - Methods to develop is FEM for moving parts, and also research Meshless method for engine block/parts coupled to FEM

Reviewers' Comments

- **A reviewer said that it is not clear if this project can achieve the goal of software development for advanced ICE modeling satisfying industries. The reviewer said that mesh generation seems like old technology, and key physical and chemical models such as spray, combustion, and engine-out emissions, are not clearly directed.**
  - *As clearly demonstrated in this presentation, the grid generation process is new, a new paradigm in grid generation, modular topology, overlaying parts. We have implemented ChemKin-Pro and will implement LLNL's Zero-RK. We've invented a new predictive method for spray modeling. We've increased speed by 300x, we produce solutions that are proven accurate much more quickly than other KIVA-3v and 4 like codes with the same number of elements. Older KIVA and like codes don't produce the correct solutions often, even on finer grids. One thing to be robust, another to be accurate and robust. Clearly, we feel the whole project over the course of time demonstrates our work on all aspects of engine modeling, from reactive chemistry, spray modeling, grid generation, accurate solution methods, fast solution methods -**ALL THAT IS NEEDED FOR A NEW PARADIGM.***
- **A few reviewers felt technical accomplishments demonstrated in the new KIVA code are excellent. They also felt it was important to have ICE & CFD examples versus another code so others can appreciate the differences.**
  - *We greatly appreciate the acknowledgement of good technical accomplishments. This effort is a complex process; developing a new system for engine modeling that makes a great deal fewer assumptions and provides much higher accuracy, while at the same time is faster than older methods or even Finite Volume methods. The current codes in use are the product of > decade of development (e.g. Convergent started in 2002 and is not state-of-the-art and still not nearly adequate in predictability)*
  - ***Our accomplishments so far done in ~6 years with limited budgets and a couple of people**.*
  - ***We are nearing that engine modeling capability to do side-by-side comparisons with other codes and validate with experimental engine data and engine standard cases with collaborators from industry and highly qualified university professors.***
  - ***The issue is more than just submodels**. Good submodels on an inherently inaccurate solver doesn't address the problem. Properly representing flow including its boundaries and moving parts are critical to proper submodel performance as demonstrated by our new spray additions to the modeling system, with greater accuracy and fluid coupling and with our new LES and moving parts. More accurate modeling with new algorithms is being developed. We have proceeded with great emphasis and promise by using newest algorithms and leveraging our recent research in state-of-the-art methods. **Careful validation is critical** to having a software capable of predictability. We insure each portion the solver works as expected, requiring careful testing and analysis on the proper problems. **Comparisons are made of current KIVA versus the PCS FEM.** Tests conducted to date, the older KIVA does not do nearly as well as the FEM method and typically needs an **order of magnitude more cells** than the method being developed. Often older KIVA does not produce exact answers. In this report we show comparison to KIVA on a benchmark problem where KIVA-4 fails (shown in the past too). We've been comparing with Convergent in an informal collaboration to understand issues with Convergent.*
- ***A reviewer suggested we do more spray modeling and engine modeling, some in the ECN Network.***
  - *We doing just this, with new spray modeling in greater detail to be predictive, are adding KH-RT to RT, and are beginning to participate in the ECN now with our John Deere and Oakland University partners. They are also going to be collaborating with us on Engine modeling and V&V of ICE modeling. It takes a great deal of effort to develop the methods from scratch to the point where we are able to do engine modeling. Some reviewers might not understand the complexity involved in this process, for example, KIVA-II started with the merging of 2 codes that had been under development for 10 years, SALE-3D and Conchas. Even then it took 4 people years to make KIVA-II. We are doing this with much less in a faster time period.*
- ***Many reviewers wondered how this might benefit more than just university researchers, how would it be supporting industry's needs, and in the hands of industrial users.***
  - *We greatly appreciate this comment and have taken many things in the development process to meet many different requirements of the code. One requirement is open source, another is the ability to support industrial users. The design of the code allows for just this, university and industry access to the source code, yet because the code is levelized, much of the inner workings should never be adjusted are underneath, allowing for commercialization of the software.*

  LANL is working on the commercialization of the software: deciding which partners best suit industries needs and fit all goals. LANL can't say who they are considering. I do not have any control over the commercialization process. I only offer advice. LANL's business and technical transfer teams handle all of business planning and legalities involved along with negotiations.

LANL & collaborations, KIVA-hpFE Development Team

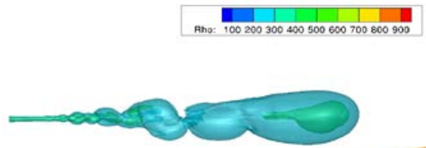
Breakdown of efforts for the code and model components

1) ***Fast grid generation*** **- CAD to CFD** grid in nearly a single step
   Dr. Carrington and Brad Philipbar (GRA) and GridPro, Inc.
2) ***New FEM Solver algorithm and code for turbulent multi-species for all-speed flows***
   Dr. Carrington
3) ***Conjugate Heat Transfer*** **is essentially free and seamless**
   Dr. Carrington and Waters
4) ***Local ALE - Mesh never tangles, robust 2nd order accurate*** **moving parts**
   Drs. Heinrich, Waters, Mazumder, Carrington and Mr. Dominic Munoz
5) ***hp*-adaptive FEM – exponentially grid convergent & evolving error drives the approximation**
   Drs. Wang, Waters and Carrington
6) **MPI with for massively parallel processing, from small clusters to LANL sized supercomputers**
   Drs. Waters and Carrington
7) **Dynamic LES turbulence modeling for all flow speeds (transition to turbulence)**
   Dr. Waters and Carrington
8) ***2nd Order accurate multi-component Spray model***
   1) ***Accurate even on coarser grids***
   2) ***Volume of Fluid (VOF) for initial spray break-up and wall films***
   Drs. Waters, Francois, and Carrington
9) **Better RANS *k-ϖ* turbulence modeling**
   Dr. Carrington
10) **Plasma Spark Model applied at an element node**
   Dr. Carrington

Future or Ongoing effort in FY17 to FY 19

- Combustion and Reactive Chemistry (ongoing)
  - *Incorporate LLNL* fast chemistry system
  - ChemKin-Pro testing V&V in KIVA-hpFE
  - Combustion and Engine V&V (collaborating with John Deere and Oakland University)
- Conjugate heat transfer between combustion chamber rest of engine
  - FEM system development for solid and moving parts (ongoing)
  - FEM coupled to BEM method for solid and moving parts (ongoing)
- Parallel *hp*-adaptive PCS FEM in 3-D (ongoing)
  - MPI on the *hp*-adaptive modules
  - OpenMP embedded in MPI Parallel constructions (MPI, enhanced by OpenMP)
- Engine Modeling with KIVA-hpFE (ongoing)
  - ***Full engine system, port, valves and piston***
  - More effort on *hp*-adaptation inclusive of moving parts
- LES Turbulence modeling development (ongoing)
  - **Dynamic LES tested in engine modeling**
  - Other turbulence closure (future Reynolds Stress Modeling – 2nd moment methods)
- Grid Generation with modular GridPro and overset parts (ongoing)
- Spray model development in FEM (ongoing)
  - Two-phase turbulence modeling with interface tracking
  - VOF allows ligaments in flow by true stress modeling
  - VOF hand-off to particle transport and engineering models

Any proposed future work is subject to change based on funding levels



Summary

New Methods and Models – *achieving robust, effective, efficient, & accurate Engine Modeling*

2017 DOE Merit Review

FEM for with Turbulence Reactive Flow with sprays

- ***Dynamic LES model***
- ***Implicit Solver system for viscous and diffusion terms in all physics equations ~ 1000x larger dt***
- ***Predictive Spray Break-up in a true multi-phase flow model***
  - ***incorporating stressing forces into Navier-Stokes using VOF***
- ***ChemKin-Pro links developed in collaboration with ANSYS Inc.***
- ***KIVA-hpFE much faster than KIVA-4 and far more accurate***
- ***Accurate droplet transport modeling***
- ***k-ϖ turbulence***
- ***Conjugate Heat Transfer proven and partially implemented***

Grid Generation *for KIVA-hpFE and KIVA-4, KIVA-3v Finite Volume*

- ***Fast Grid Generation, in collaboration with GridPro Inc.***

hp-adaptive FEM

- ***hp-adaptive FEM incorporated in the 3D PCS FEM all flow solver with some benchmarking (V&V)***
- Higher order accurate - greater spatial accuracy everywhere & always
- *Evolving solution error drives grid*

Local ALE in FEM

- ***2nd order accurate and the Mesh never tangles***
- ***Only 1% of solution time is spent on grid movement***
- ***Faster grid generation*** - CAD to CFD grid in nearly a single step

RED highlight bulleted subjects were discussed today

Parallel Solution

- ***MPI processing*** ***for great solutions on moderate computer platforms.***
- ***Much Faster than KIVA-4 parallel and 300x to 450x faster*** ***than our serial versions of KIVA.***
- ***Parallel Spray and Moving Parts system***

Technical Back-Up Slides

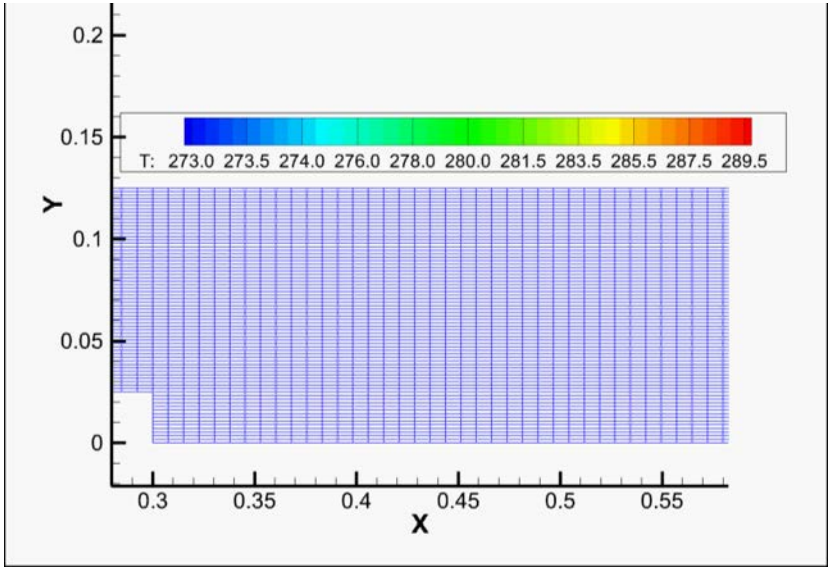
Dynamic LES for Wall Bounded Flows

Backward-facing step Re=27,000
Pr = 0.71, Air at 273 deg K
Incompressible flow

Convective flow: heat flux determines wall temperature.

- This is similar to the Conjugate Heat Transfer. Here heat flux is prescribed at the wall, rather than solving for it too.

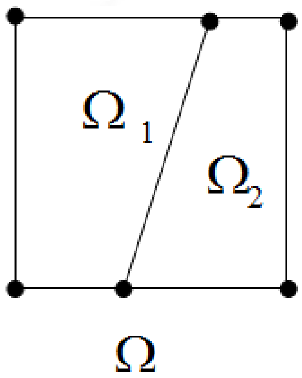
Compares well to experimental data of Vogel and Eaton as shown in the previous slide.

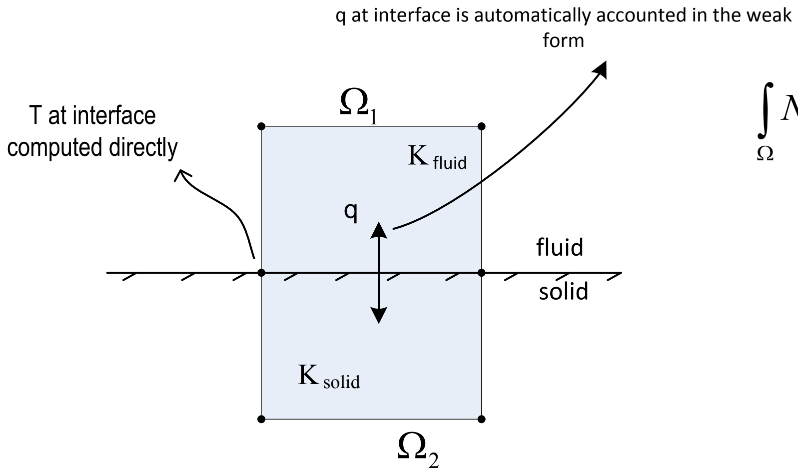


View is only around the step's vicinity

Internal Energy Transport with Conjugate Heat Transfer

- **Eliminates need for heat transfer coefficient**
- **All the temperatures to be computed directly, heat flux automatically preserved.**
- Simple process when nodes are shared and easy for an interface element of moving solid and fluid.
  - Ω the interface element, Ω_1 **fluid**, Ω_2 **solid**
  - Energy and T at all nodes of solid, liquid and interface are calculated
  - Energy is advected at fluid nodes, convective heat transfer
  - Accurately establishes the temperatures and heat flux

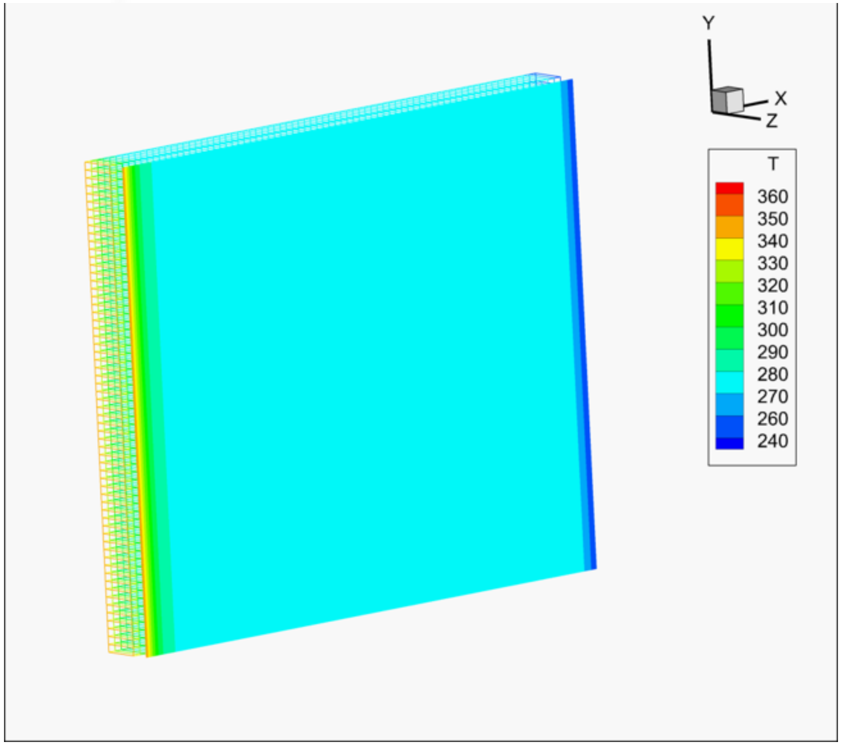




$$\int_{\Omega} N_i R(T_i)\, d\Omega = \int_{\Omega_1} N_i R(T_{1_i})\, d\Omega_1 + \int_{\Omega_2} N_i R(T_{2_i})\, d\Omega_2$$

Conjugate Heat Transfer

Differentially Heat Cavity filled with Air 279 K°



Steel case:

- 2 sides with fixed temperature
- Code identifies Solid and Fluid type Cells
- Standard boundary condition types:
    - Fixed temp walls outer walls
    - Fixed no-slip inner walls

Heat/Energy Conduction is solved in solids
Momentum, Energy, Species, Chemistry solved in fluids

Spark Kernel Model

- Heat from spark as function of time to *mimic* solution of Spark Kernel
  - Spark wattage as function of time (from ignition specification)
    - Discrete empirical model applied
    - 5 averaged pieces from the experimental values in J/s
  - Kernel heat loss as function of time from heat transfer mechanisms
  - Spark energy applied at single point (node) and processed through the momentum and energy equations before chemistry solve

Governing Eq. Spark Plasma Kernel

$$\frac{dU}{dt} = \frac{dW}{dt} + \frac{dQ_{chem}}{dt} - \frac{dQ_{loss}}{dt} - p\frac{dV_k}{dt}$$

$$\frac{dT_k}{dt} = \frac{1}{m_k c_{p,k}}\left(\frac{dW_{spark}}{dt} + \left(h_{chem} - h_k\right)\rho\, A_k S_{eff} - \frac{dQ_{loss}}{dt} + V_k\frac{dP}{dt}\right)$$

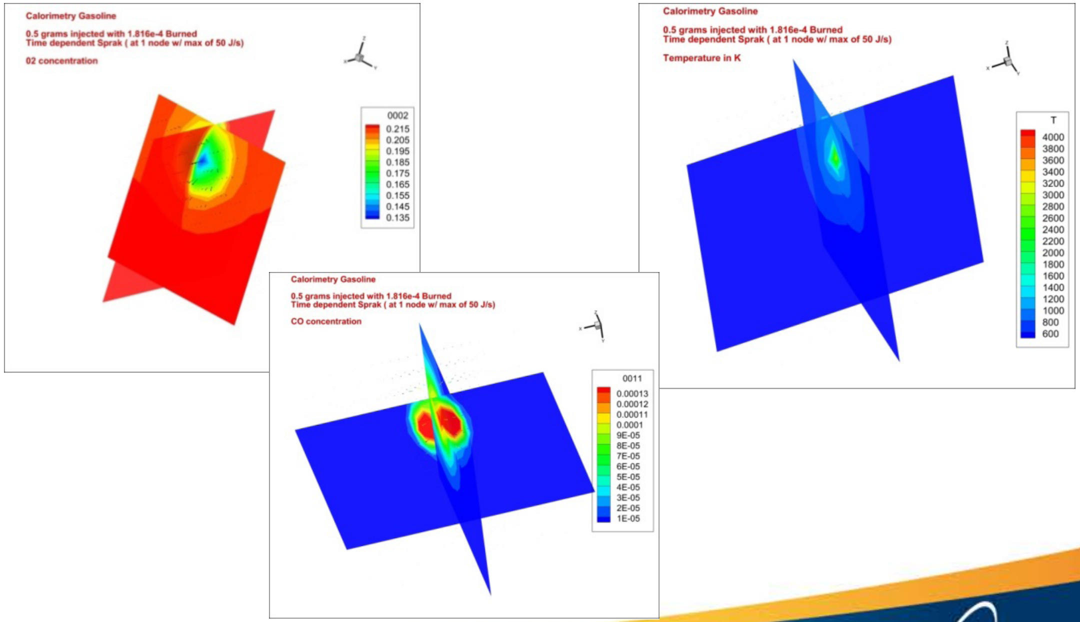
$$\frac{dV_k}{dt} = \frac{\rho_f}{\rho_k} A_k S_{eff} + V_k\left(\frac{1}{T_k}\frac{dT_k}{dt} - \frac{1}{P}\frac{dP}{dt}\right)$$

$$\frac{dr_k}{dt} = \frac{\rho_f}{\rho_k} S_{eff} + \frac{V_k}{A_k}\left(\frac{1}{T_k}\frac{dT_k}{dt} - \frac{1}{P}\frac{dP}{dt}\right)$$

$$\frac{dh_k}{dt} = c_{p,k}\frac{dT_k}{dt} \qquad S_{eff} = S_{flame} + S_{heat\_diff}$$

Velocity of Flame + Heat diffusion

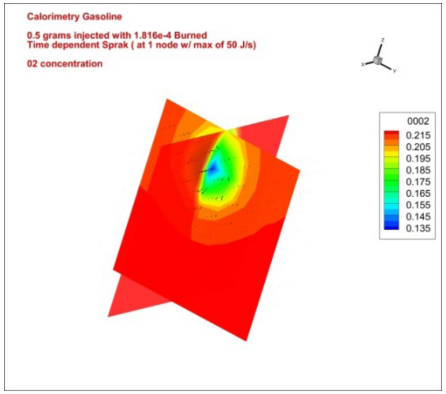
- Calorimetric validation to LHV
  - 0.5 grams Gasoline (KIVA) at 325K injected into Air at 1atm & 296 K
  - Spark at node at max of 50 J/s

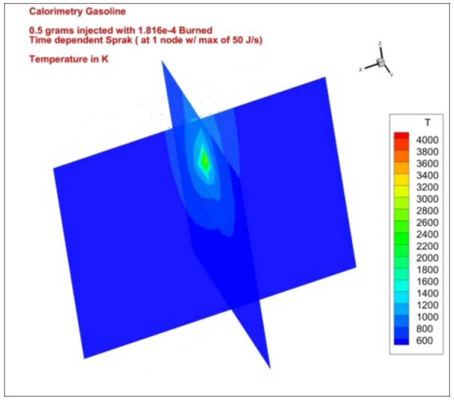


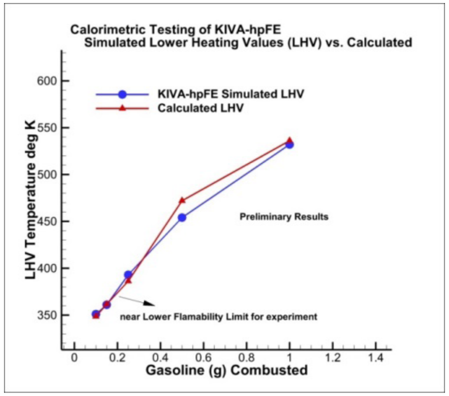
UNCLASSIFIED

Spark/Flame Kernel Approximation Model

- Spark Heat Transfer - $f(\Delta t)$
  - Spark wattage as function of time (from ignition specification)
    - Discrete empirical model applied $\Delta t >> dt$
    - 5 averaged pieces from the experimental values in J/s
  - Kernel heat loss as function of time
    - Discrete model based on reported solution to equations $\Delta t >> dt$
    - 5 averaged pieces from the Plasma kernel model equation results in J/s
  - Spark energy applied at single point (node)
    Then solve momentum and energy equations before chemistry solve







- Calorimetric validation to LHV
  - Gasoline (KIVA) at 325K injected into Air at 1atm & 296 K
  - Spark at node at max of 50 J/s

UNCLASSIFIED